

Supporting Information

Initial Decomposition Reaction of Di-tetrazine-tetroxide (DTTO) from Quantum Molecular Dynamics: Implications for a Promising Energetic Material

Cai-Chao Ye,^{†,‡} Qi An,[†] William A. Goddard, III ^{,†} Tao Cheng,[†] Wei-Guang Liu,[†] Sergey V. Zybin,[†] and
Xue-Hai Ju [‡]*

[†]Materials and Process Simulation Center, 139-74, California Institute of Technology, Pasadena, California
91125, United States

[‡]Key Laboratory of Soft Chemistry and Functional Materials of MOE, School of Chemical Engineering,
Nanjing University of Science and Technology, Nanjing 210094, P. R. China

*E-mail: wag@wag.caltech.edu

Table of Contents:

Page 3: Coordinates for structure of c1-P212121 DTTO

Page 4: Coordinates for structure of c2-Pbca DTTO

Page 5: Figure S1. Supercell of the DTTO crystal: (a) c1-P212121 DTTO supercell; (b) 30% compressed c1-P212121 DTTO supercell; (c) c2-Pbca DTTO supercell.

Page 6: Figure S2. Single point energy and the distances between the nearest two N atoms of two c2-DTTO during the two DTTO combine reaction. Time step is 0.005 ps.

Page 7: Table S1. The bond type and bond cut-off table in the fragment analysis.

Page 8: Table S2. Single point energy and the distances between the nearest two N atoms and the nearest two O atoms of two c2-DTTO during the two DTTO combine reaction.

Page 9: Atomic coordinates of all intermediates and TS shown in this study.

Coordinates for structures of c1-P212121 DTTO

```

_pd_phase_name          'P212121'
_cell_length_a          18.12900
_cell_length_b          5.39900
_cell_length_c          6.93650
_cell_angle_alpha       90
_cell_angle_beta        90
_cell_angle_gamma       90
_symmetry_space_group_name_H-M  'P 21 21 21'
_symmetry_Int_Tables_number 19

```

```

loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
  '-x+1/2, -y, z+1/2'
  '-x, y+1/2, -z+1/2'
  'x+1/2, -y+1/2, -z'

```

```

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
O1      1.0      0.246910      0.264340      0.587080      Uiso  0.012670 O
O2      1.0      0.102870      0.603520      0.587820      Uiso  0.012670 O
O3      1.0      0.996090      0.627930      0.954250      Uiso  0.012670 O
O4      1.0      0.139860      0.287530      0.955810      Uiso  0.012670 O
N1      1.0      0.114150      0.106390      0.041840      Uiso  0.012670 N
N2      1.0      0.068100      0.955990      0.946750      Uiso  0.012670 N
N3      1.0      0.040560      0.755330      0.046010      Uiso  0.012670 N
N4      1.0      0.058000      0.688340      0.226020      Uiso  0.012670 N
N5      1.0      0.180640      0.212520      0.321540      Uiso  0.012670 N
N6      1.0      0.200870      0.140450      0.496950      Uiso  0.012670 N
N7      1.0      0.175190      0.933870      0.595070      Uiso  0.012670 N
N8      1.0      0.127270      0.787510      0.503190      Uiso  0.012670 N
C1      1.0      0.604660      0.657500      0.687920      Uiso  0.012670 C
C2      1.0      0.634450      0.443480      0.764430      Uiso  0.012670 C

```

Coordinates for structures of c2-Pbca DTTO

```

_pd_phase_name          'Pbca'
_cell_length_a          25.54000
_cell_length_b          5.43300
_cell_length_c          9.68500
_cell_angle_alpha       90
_cell_angle_beta        90
_cell_angle_gamma       90
_symmetry_space_group_name_H-M  'P b c a'
_symmetry_Int_Tables_number  61

```

```

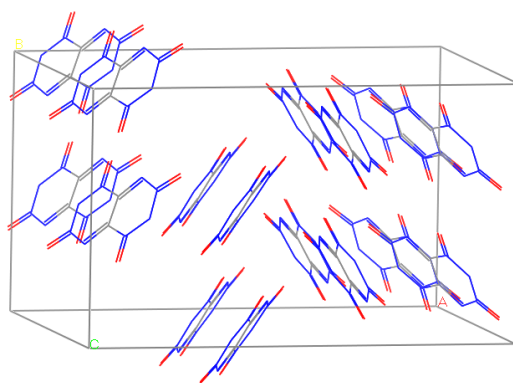
loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
  '-x, -y, -z'
  '-x+1/2, -y, z+1/2'
  'x+1/2, y, -z+1/2'
  '-x, y+1/2, -z+1/2'
  'x, -y+1/2, z+1/2'
  'x+1/2, -y+1/2, -z'
  '-x+1/2, y+1/2, z'

```

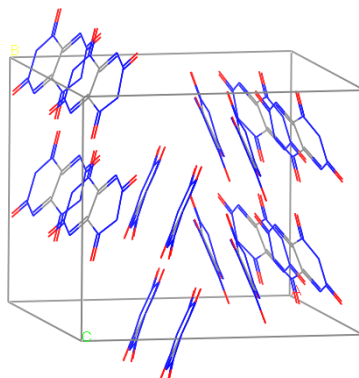
```

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
N1      1.0      1.095850      0.117770      0.356090      Uiso  0.012670 N
N9      1.0      1.051590      0.000100      0.391960      Uiso  0.012670 N
N17     1.0      1.040920      0.783530      0.322700      Uiso  0.012670 N
N25     1.0      1.068020      0.685780      0.218880      Uiso  0.012670 N
N33     1.0      1.174470      0.134050      0.212760      Uiso  0.012670 N
N41     1.0      1.203250      0.035990      0.109370      Uiso  0.012670 N
N49     1.0      1.182320      0.834500      0.043310      Uiso  0.012670 N
N57     1.0      1.138790      0.713100      0.077740      Uiso  0.012670 N
C1      1.0      1.127300      0.026000      0.251190      Uiso  0.012670 C
C9      1.0      1.111410      0.810590      0.183080      Uiso  0.012670 C
O1      1.0      1.001620      0.675430      0.364430      Uiso  0.012670 O
O9      1.0      1.106410      0.307360      0.421930      Uiso  0.012670 O
O17     1.0      1.192470      0.320290      0.268590      Uiso  0.012670 O
O25     1.0      1.207650      0.761520      0.943290      Uiso  0.012670 O

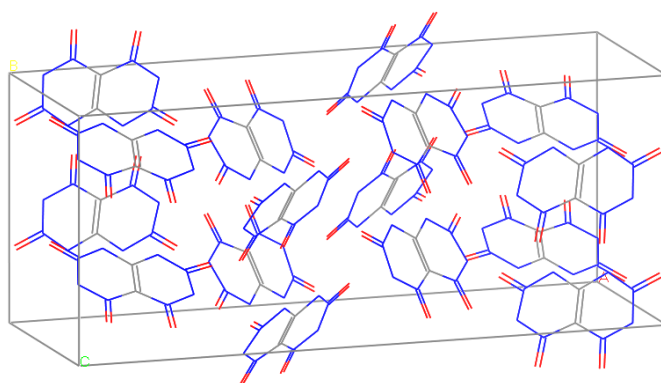
```



(a) c1-P212121 DTTO supercell



(b) 30% compressed c1-P212121 DTTO supercell



(c) c2-Pbca DTTO supercell

Figure S1. Supercell of the DTTO crystal: (a) c1-P212121 DTTO supercell; (b) 30% compressed c1-P212121 DTTO supercell; (c) c2-Pbca DTTO supercell.

Single point energy and N-N distance

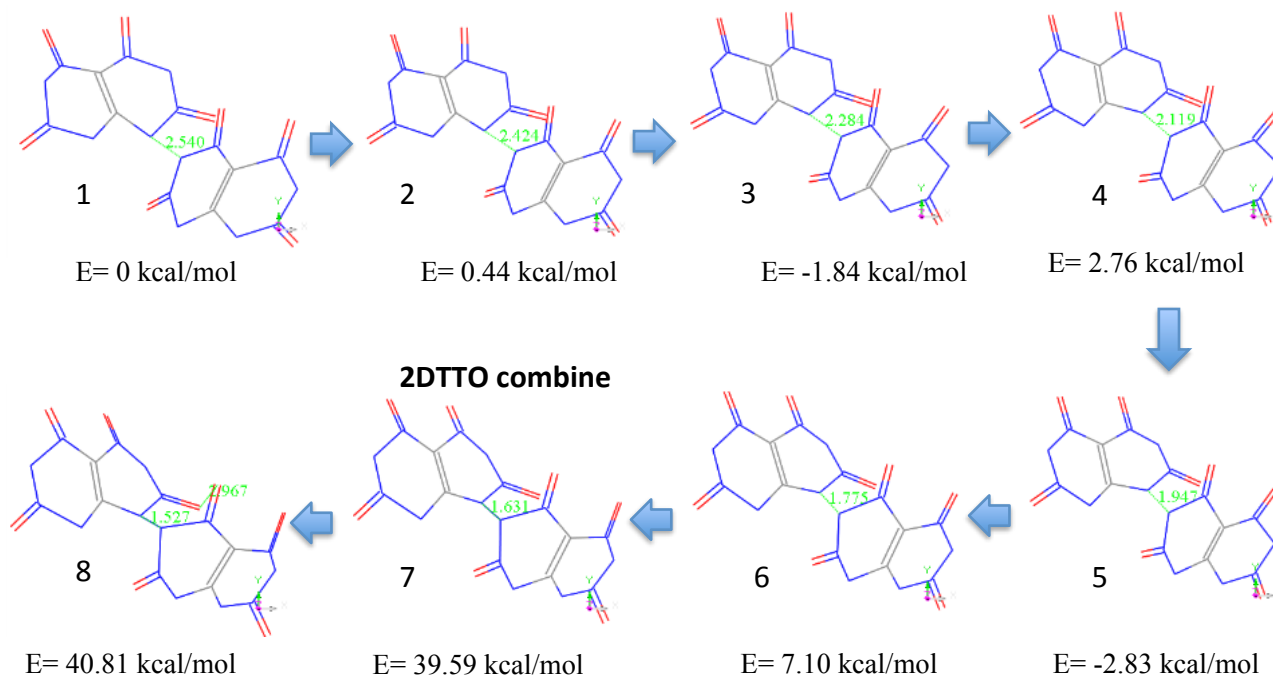


Figure S2. Single point energy and the distances between the nearest two N atoms of two c2-DTTO during the two DTTO combine reaction. Time step is 0.005 ps.

Table S1. The bond type and bond cut-off table in the fragment analysis.

Bond type	rcut-off (Å)
C-C	2.31
C-O	2.15
C-N	2.20
O-O	2.22
O-N	2.10
N-N	2.17

Table S2. Single point energy and the distances between the nearest two N atoms and the nearest two O atoms of two c2-DTTO during the two DTTO combine reaction.

Steps	Total Energy (a.u.)	Relative single point energy (kcal/mol)	N-N distance (Å)	O-O distance (Å)
1	-1627.64747	0	2.540	2.647
2	-1627.64676	0.44	2.424	2.729
3	-1627.65040	-1.84	2.284	2.771
4	-1627.64306	2.76	2.119	2.804
5	-1627.65196	-2.83	1.947	2.830
6	-1627.63615	7.10	1.775	2.865
7	-1627.58437	39.59	1.631	2.921
8	-1627.58172	40.81	1.527	2.967

Atomic coordinates of all intermediates and TS shown in this study:

TS1

&zmat

O2	2.2843647163000	2.9860514004000	3.8483334456000
N3	0.4876706036000	3.6098626133000	0.6855217405000
N4	0.7376718664000	3.8702225381000	1.8721265478000
N7	3.2968333423000	4.9601079123000	4.1441749934000
N8	2.4232886012000	4.1592413222000	3.4543577145000
C7	1.7755013799000	4.6545696798000	2.3197117754000
O3	-0.4547663592000	3.2232910796000	0.0517960752000
N2	1.6344598597000	4.9402519125000	-0.7836127770000
O4	2.4347233315000	7.1258258409000	-0.7050871739000
O1	4.3219176980000	6.9156089218000	4.2140753116000
N1	2.0240400488000	6.0143583868000	-0.4797471521000
N5	3.1826011500000	6.5806432944000	2.2455894364000
N6	3.6366939363000	6.1364078101000	3.5660297182000
C8	2.2321880573000	5.8423201579000	1.7737484275000

b:

&zmat

O2	2.4230193830000	3.3088639716000	2.8250250819000
N3	0.3214654431000	3.2359900821000	1.3010016552000
N4	0.1703790492000	4.4036624803000	1.8731315538000
N7	3.1008710675000	5.3646387951000	3.5790728510000
N8	2.2660872139000	4.5433492773000	2.9574384634000
C7	1.1145084916000	5.1645738185000	2.3558228687000
O3	-0.3561048735000	2.2537341287000	1.4559806185000
N2	2.9977633344000	5.1211311386000	0.0953377369000
O4	3.1980185676000	6.8545494891000	-1.4721038818000
O1	5.2639454845000	5.4460753504000	4.0684554331000
N1	3.0933538695000	5.9725938984000	-0.6712601906000
N5	0.9525514885000	7.7530504618000	2.2167393737000
N6	4.4161373407000	5.0134305287000	3.3282385330000
C8	1.0551923721000	6.5831194497000	2.2941379863000

TS2:

&zmat

O2	2.6492336541000	3.5376014598000	2.3607930006000
N3	0.4284345605000	3.4110747199000	1.2791319489000
N4	0.0950480503000	4.4269629841000	1.9980751881000
N7	3.1802823909000	5.4993451307000	3.7137050781000
N8	2.3033600698000	4.6559047904000	2.7595535886000
C7	1.0602373907000	5.1745833434000	2.5891903157000
O3	-0.2569195297000	2.4714017083000	0.9458873192000
O1	5.4027922211000	5.8805278508000	3.8528406851000
N5	0.4874037907000	7.6096302399000	3.2915246299000
N6	4.3739263966000	5.4693637940000	3.3417296663000
C8	0.7820824805000	6.5123184141000	2.9863439387000

c:

&zmat

O2	2.0934156612000	3.4346861772000	1.7840888288000
N3	0.3791791142000	3.2902780713000	1.4925624673000
N4	-0.0762332835000	4.4014376488000	1.8994333906000
N7	3.7070828214000	6.0604175863000	4.7622978422000
N8	2.1740218391000	4.6177273996000	2.2951546422000
C7	0.9714306372000	5.1825593024000	2.3707138993000
O3	-0.0692852539000	2.2876087965000	1.0103942329000
O1	5.4548587182000	5.5167737592000	3.2912058705000
N5	0.5553215219000	7.5730001271000	3.2887282997000
N6	4.5639897378000	5.7948419415000	4.0441284096000
C8	0.7520999621000	6.4893836254000	2.8800674759000

TS1'

&zmat

O29	8.3272476659	6.7588673412	3.6862760220
O30	6.0384470908	10.3913244833	4.7855533030
O32	9.1089912462	6.9045866250	8.5190682006
O57	11.0103786546	8.7528095364	5.3865885808
O58	12.8166440265	5.4900178937	7.7640894879
O59	10.8161834366	6.2082826714	12.0965524692
O60	9.9179433084	9.8901253664	9.8064683365

N57	7.7014360650	7.6401827596	8.1312829929
N58	7.2547145160	8.4211628222	9.0706285844
N59	6.8978731066	9.7571614858	8.6611686354
N60	6.6157646272	10.0801218950	7.3891053939
N61	8.1005939593	7.0721832129	5.8750196936
N62	7.8737382410	7.4457380965	4.5980431371
N63	7.1225400959	8.5482170980	4.1709592842
N64	6.6824887735	9.3930157097	5.1265708917
N113	10.1622494696	8.6854678321	9.8803853206
N114	10.3704296887	8.1243314918	11.0602154149
N115	10.8809802408	6.8198874594	11.0297475335
N116	11.5496643485	6.2679202667	9.9903941156
N117	10.3231174723	8.6879914017	7.4869088859
N118	11.0164466351	8.1951011835	6.4874250754
N119	11.8461628998	7.0287637897	6.4893430416
N120	12.0087900575	6.4255778417	7.6730890175
C9	6.9637503579	9.1434200519	6.5025082964
C10	7.6173586623	7.9344465804	6.7770154664
C27	11.2890653837	6.8512458820	8.8332620045
C28	10.2288176343	7.8226482660	8.5912639083
O31	6.7602742611	10.5703553932	9.5642766737

b':

&zmat

O29	8.0816757765000	6.4110149396000	3.7522751827000
O30	7.0748069095000	10.6845638112000	4.3736285517000
O32	9.8323549324000	6.3987933204000	8.9291588785000
O57	10.1631734978000	8.8525828962000	5.7389808346000
O58	12.7212627058000	5.6439312172000	7.3952774553000
O59	12.3285880942000	6.4631082621000	12.1272225875000
O60	9.4079326140000	9.3619292330000	10.4525120760000
N57	6.9660873396000	7.6591852727000	7.9774815820000
N58	6.6833814500000	8.5086342569000	8.8283718502000
N59	6.6090166536000	10.0839566494000	8.2743517234000
N60	6.7661037194000	10.3708794474000	7.0053159481000
N61	7.5367200652000	6.9388773912000	5.8446677955000
N62	7.7226036594000	7.2741245163000	4.5543165475000
N63	7.5254375398000	8.5419074645000	3.9912515154000
N64	7.2179469653000	9.5466947354000	4.8366429162000

N113	10.1481857856000	8.3819766893000	10.3230033882000
N114	10.7852648894000	7.8819035518000	11.3567774988000
N115	11.7778777831000	6.7970476191000	11.0905000476000
N116	12.0860333816000	6.2656544398000	9.9358904231000
N117	9.9649243681000	8.6436429392000	7.9300799981000
N118	10.4706933520000	8.2733297891000	6.7800114061000
N119	11.4324805227000	7.2065393642000	6.5154282865000
N120	11.8428741386000	6.4922524000000	7.5459515525000
C9	7.0506036147000	9.2983676860000	6.2306689350000
C10	7.1927312574000	7.9769886814000	6.6299890276000
C27	11.2509994863000	6.6757051497000	8.9109747986000
C28	10.2756491794000	7.7699021571000	8.9635849223000
O31	6.3866822437000	10.9074605570000	9.1388940383000

TS2'

&zmat

O32	9.8958149290	5.8692298655	8.9071388816
O57	10.4125413508	9.0826881686	5.8131253844
O58	12.4045846466	5.4124487418	7.1629240887
O59	12.6778709789	6.6946686930	11.8867405798
O60	9.1674675734	9.0327307634	10.4870635119
N113	10.0819965589	8.2164781146	10.3150712475
N114	10.7279705574	7.6820971911	11.3201905559
N115	11.9273014999	6.7986284647	10.9266585714
N116	12.1059345975	6.2099178605	9.7955005003
N117	10.1643964685	8.6965627871	7.9848607071
N118	10.6601891924	8.3347902625	6.7486103949
N119	11.3962459051	7.2053276562	6.4049113501
N120	11.7151311217	6.3865236827	7.4151309868
C27	11.0421897532	6.5096611190	8.8728569261
C28	10.4797815272	7.8610297215	8.9391307265

c'

&zmat

O32	9.8718459679000	5.6397367170000	8.3280057292000
O57	9.2708933818000	7.9462670877000	6.1443644511000
O58	13.4512682219000	6.6565512251000	6.6367603019000
O59	12.1099944043000	6.1981945646000	12.1860735751000
O60	10.3394898276000	9.7711166169000	10.3017252987000

N113	10.6493819014000	8.5762072712000	10.2904282896000
N114	11.0752531279000	7.9918159920000	11.3880799772000
N115	11.4401607113000	6.5774186574000	11.2327916462000
N116	11.0434677404000	5.7492490135000	10.2976672434000
N117	10.4337359373000	8.5382830010000	7.9769887422000
N118	10.3491461231000	7.8302255360000	6.7093127509000
N119	11.4139235962000	7.3405680923000	6.1383335487000
N120	12.4414463276000	7.0623191432000	7.1443063691000
C27	10.4378472864000	6.3108574067000	9.1847196955000
C28	10.5315621053000	7.8039727678000	9.0203567943000

c''

&zmat

O32	10.7606539918	5.2794318840	8.1852696921
O57	9.1999246042	7.3080144969	6.6885052965
O58	12.8384271733	7.9167787557	6.6832116945
O59	10.6328147954	6.2395156182	12.5806113394
O60	11.7850795069	9.4888414741	9.8177602299
N113	11.3870428679	8.3294183414	10.0158059860
N114	11.3060719686	7.8812354055	11.2656692816
N115	10.8310698513	6.5276565561	11.4015191336
N116	10.6620177943	5.6196536203	10.4571586785
N117	11.0659920939	8.0505269666	7.7275559819
N118	10.4139762259	7.4309596425	6.6966973240
N119	11.1202683124	7.2454007646	5.4683175829
N120	12.3558328393	7.5920855231	5.5773410744
C27	10.8043994264	6.0457085587	9.1505277356
C28	11.0020511583	7.5008200462	8.9126031097

TS3'

&zmat

O32	10.1452441044	5.5009404107	8.7158500168
O57	9.6300855642	8.5032355805	5.7860655425
O58	12.8836666062	5.8836847129	7.1619605300
O59	12.0469695366	6.0487980655	12.1778162648
O60	10.4720925501	9.7638962937	10.3679747920
N113	10.4109815442	8.5070335277	10.2796556257
N114	10.1299528105	7.6668910030	11.1867302784
N115	11.8823636536	6.2578571343	11.0156102663

N116	12.2296869320	6.1830762956	9.8735318702
N117	10.1989293022	8.6184599756	7.9448367281
N118	10.3419289971	8.0742673978	6.6852177642
N119	11.4135031426	7.2764916192	6.2984890483
N120	11.9098839618	6.5997462703	7.3321158832
C27	10.9059866679	6.4487432567	8.7981096837
C28	10.5478100820	7.8829665538	8.9591994980

TS3''

&zmat

O32	10.5738620628	5.2876803337	8.2134304054
O57	9.1829935526	7.2791492865	6.5372619152
O58	12.8732106680	8.0662638145	6.7190872759
O59	10.7603615405	6.2354810212	12.6104009938
O60	11.8203131714	9.4571195909	9.7753870687
N113	11.4007003113	8.3098810267	10.0000625707
N114	11.3728844832	7.8680759953	11.2573994078
N115	10.8897957702	6.5263814788	11.4217835171
N116	10.6446524820	5.6206909730	10.4884760643
N117	10.9447067436	8.0358506811	7.7336626631
N118	10.3787355416	7.3761420330	6.7150585068
N119	11.2820614666	7.2012315524	5.4116984180
N120	12.4189564045	7.6478758514	5.6386883727
C27	10.7011104562	6.0479482163	9.1780315119
C28	10.9216719836	7.4965904666	8.9278213245

d'

&zmat

O32	9.5662683232000	5.2055726862000	9.0106151287000
O57	11.8813862405000	9.3238760336000	6.7541225179000
O58	11.5992164023000	4.9380860908000	7.2996659023000
O59	14.7580907460000	7.3041729735000	10.7687641345000
O60	9.4650518069000	8.1415389244000	11.3756702960000
N113	9.1790914516000	7.9157824942000	10.2173077784000
N114	8.2714745244000	7.8888984047000	9.3411704902000
N115	13.6194267249000	7.2212051604000	10.4181605218000
N116	12.5243077990000	7.1413674410000	10.0805335884000
N117	10.2703819208000	8.6810899963000	8.1292698600000

N118	11.2681227600000	8.4242342618000	7.3324193997000
N119	11.7988024236000	7.1121790512000	6.9650623520000
N120	11.2250667086000	6.0857163935000	7.5451239828000
C27	10.0323946725000	6.2150693363000	8.5566320453000
C28	9.6842448026000	7.6155638332000	8.7910316148000

d''

&zmat

O32	9.9158451729	5.7261034048	8.0204899669
O57	8.5871694028	7.0122818062	6.2622705438
O58	14.4273366869	7.3516740855	5.8186710984
O59	12.3458648125	5.9427221192	11.8440189938
O60	10.6704941192	9.6908233828	10.1367140494
N113	10.7923788969	8.4541006971	10.0708414772
N114	11.5405194766	7.8339202648	11.0503052015
N115	11.6853111605	6.4648428992	10.9438108462
N116	11.2013940371	5.6395519587	9.9640488213
N117	9.4844301442	8.1551613838	8.0443678259
N118	9.1933308692	7.2085326676	7.2709777440
N119	12.2928886723	7.5535962908	6.7673775797
N120	13.3390113111	7.4543722926	6.3024641627
C27	10.4691882958	6.2942880120	9.0528321608
C28	10.2243065651	7.6907931051	9.0963281231

TS4'

&zmat

O2	2.6985498278000	2.9627585195000	3.5528781190000
N3	-0.6005780941000	4.7970233741000	0.1073633423000
N4	3.5307580364000	3.7477656594000	0.8963352122000
N7	2.4375169372000	5.1173165644000	4.0636936365000
N8	2.7588601823000	4.1496492119000	3.2000463244000
C7	3.1645374852000	4.5196976184000	1.9012627014000
O3	-1.7793047022000	4.9663894063000	0.2271104953000
N2	0.5313508579000	4.6342812195000	-0.0111163098000
O4	3.8094156580000	4.6614892492000	-0.0929769137000
O1	2.1704067050000	7.2999219802000	4.4512096642000
N1	3.6212476782000	5.9872187727000	0.2863322349000
N5	2.8850266156000	6.9248732305000	2.3804780230000

N6	2.5096614979000	6.5069344099000	3.5800931453000
C8	3.2102656788000	5.8942126441000	1.5541512055000

f:

&zmat

O2	2.6985498278000	2.9627585195000	3.5528781190000
N3	-0.6005780941000	4.7970233741000	0.1073633423000
N4	3.5307580364000	3.7477656594000	0.8963352122000
N7	2.4375169372000	5.1173165644000	4.0636936365000
N8	2.7588601823000	4.1496492119000	3.2000463244000
C7	3.1645374852000	4.5196976184000	1.9012627014000
O3	-1.7793047022000	4.9663894063000	0.2271104953000
N2	0.5313508579000	4.6342812195000	-0.0111163098000
O4	3.8094156580000	4.6614892492000	-0.0929769137000
O1	2.1704067050000	7.2999219802000	4.4512096642000
N1	3.6212476782000	5.9872187727000	0.2863322349000
N5	2.8850266156000	6.9248732305000	2.3804780230000
N6	2.5096614979000	6.5069344099000	3.5800931453000
C8	3.2102656788000	5.8942126441000	1.5541512055000

TS1*

&zmat

N1	13.4060465343	5.6451432058	0.7899229243
N2	11.9792193918	5.4178723125	0.6568553208
N3	11.5788027481	4.7039826336	-0.7950687497
N4	12.4444003574	4.1214171301	-1.5369919509
N5	15.6300084404	5.0266222566	0.0897646636
N6	16.4432438096	4.1786080987	-0.5804334006
N7	15.8319993010	3.2723566436	-1.4350851141
N8	14.5370583035	3.2817681358	-1.8002513272
N9	9.1031052124	7.9678991229	-0.5340658991
N10	10.2814557573	7.9320203106	-1.2104297658
N11	11.3688172114	7.5226444682	-0.5291191455
N12	11.3451722276	6.8113578546	0.7084296123
N13	7.9082166113	7.6916470613	1.5941683057
N14	7.8225483789	7.0874228371	2.8191720703
N15	8.9038820722	6.3265633066	3.2098296452
N16	10.1120145697	6.2723615191	2.5870493575

C17	14.2242329274	4.9537729267	-0.0657616758
C18	13.7473561143	4.1177703652	-1.1074953032
C19	9.0408642176	7.4979768759	0.7893808396
C20	10.1281291493	6.8483934913	1.3857671035
O21	10.4001417334	4.8981171514	-1.0513571909
O22	13.7302639198	6.4282152412	1.6953254713
O23	16.1687402727	5.8585467317	0.8356715936
O24	12.4903038462	7.5551654213	-1.0717611407
O25	8.1017495193	8.3839904944	-1.1542063073
O26	6.9446040568	8.3834256733	1.2532536274
O27	8.7594041037	5.6974251004	4.2548299067
O28	16.5884919062	2.4299981024	-1.9292884043

b*

&zmat

N1	13.4446018876000	6.1068968454000	0.0596773331000
N2	12.1834854671000	5.8196633958000	0.5909666824000
N3	11.7266260645000	4.3887849878000	-0.8655821277000
N4	12.5584063266000	3.4575127796000	-1.1322672783000
N5	15.5900760428000	5.0581620463000	0.3028359898000
N6	16.4971917717000	4.0816241820000	0.0059275256000
N7	16.0077260688000	2.9906541168000	-0.6705596695000
N8	14.7084971535000	2.7518870070000	-0.9914873801000
N9	9.2967083797000	8.5952458405000	0.0772452553000
N10	9.4302044897000	8.1623567912000	-1.1608367367000
N11	10.5527561089000	8.6920989917000	-1.7886890401000
N12	11.3713671915000	6.8023571502000	0.5326059808000
N13	8.0605134024000	7.5072023596000	1.8514886585000
N14	7.9189984912000	6.5256358092000	2.7976822973000
N15	8.9452440722000	5.6098049808000	2.8772050317000
N16	10.1057055318000	5.6296142493000	2.1726149072000
C17	14.2547733116000	4.9581460791000	-0.1067732014000
C18	13.8528150110000	3.7425008237000	-0.7103675588000
C19	9.1915697166000	7.5630542657000	1.0548935403000
C20	10.2086304393000	6.6193977916000	1.2686818216000
O21	10.5491630239000	4.4660709255000	-1.0990287478000
O22	13.8876589408000	7.2552637801000	-0.0453115510000
O23	16.0060535581000	6.0162719388000	0.9655485385000

O24	10.6453840710000	8.5569957145000	-2.9805733137000
O25	9.2816624520000	9.7975444637000	0.4201706577000
O26	7.1249320878000	8.3123434083000	1.7312982131000
O27	8.7775656727000	4.7018481486000	3.6930263243000
O28	16.8419559584000	2.1435455997000	-0.9822870857000

TS2*

&zmat

N1	13.4704548742	5.1986847253	0.5578259774
N2	11.9675192758	5.1143268191	1.4365242769
N3	12.6431130175	3.8786364067	-0.8487657881
N4	13.1759117312	2.7311941587	-0.6160398488
N5	15.3209640791	4.3172546262	1.8906263633
N6	16.1147616775	3.2503362375	2.2466919273
N7	15.8243176178	2.0470369776	1.6419675520
N8	14.8733333025	1.8118211990	0.6880824926
N9	9.4642947296	7.7754152464	0.0048390533
N10	9.7863466161	6.8215692460	-0.8383205603
N11	10.5564185172	7.4121447458	-1.9058243685
N12	11.5372913698	6.2479259256	1.3411430891
N13	8.2603715973	7.7389843361	2.1041778128
N14	8.1661799475	7.4577932316	3.4450363773
N15	9.2016620182	6.7511390074	3.9937174252
N16	10.2954737454	6.2625426277	3.3235039171
C17	14.3115983457	4.1457438380	0.9701419789
C18	14.1368877722	2.8821527360	0.3848371446
C19	9.3821562204	7.3576978789	1.3718491247
C20	10.3445144877	6.5904795036	2.0325499857
O21	11.7683485449	4.1690519300	-1.6259308560
O22	13.8445673634	6.3229098149	0.2537117291
O23	15.5529246626	5.4010154385	2.4458011526
O24	10.5588123768	6.7948565242	-2.9324623787
O25	9.2416160402	8.9706498508	-0.2824208360
O26	7.3018071540	8.3302321296	1.5933296151
O27	9.1198890830	6.5164189678	5.1969874656
O28	16.5178653187	1.0980420764	2.0025307547

c*

&zmat

N1	13.4138571931000	5.0475741001000	0.2707968086000
N2	11.4706064616000	4.5077351972000	1.2424471962000
N3	13.0061592582000	3.9795792424000	-1.1068639971000
N4	13.5551453713000	2.8286614619000	-0.9135019062000
N5	15.0591770727000	4.3953076870000	1.9888258843000
N6	15.8569147139000	3.3793289045000	2.4558232919000
N7	15.8329391389000	2.1916562076000	1.7458398996000
N8	15.0963872381000	1.9123932512000	0.6259921190000
N9	9.5550626054000	7.7360834387000	0.0622146623000
N10	9.6528865714000	6.7261754510000	-0.7726021652000
N11	10.4822364454000	7.1624388801000	-1.8832973777000
N12	11.1751670113000	5.6467335798000	1.3261438403000
N13	8.5180776943000	8.0330111355000	2.2333255966000
N14	8.4412693358000	7.7934264613000	3.5867084107000
N15	9.2679119371000	6.8230387405000	4.0816815756000
N16	10.1108465133000	6.0244509534000	3.3469728871000
C17	14.3316208686000	4.2025868103000	0.8389004316000
C18	14.3619107423000	2.9422339101000	0.2152169140000
C19	9.4386146047000	7.3557191929000	1.4364981555000
C20	10.1637704761000	6.3321538206000	2.0514304437000
O21	12.2329147134000	4.3664342822000	-1.9453149961000
O22	13.2893072985000	6.2654091054000	0.2299945918000
O23	15.0309105724000	5.4580176746000	2.6355083598000
O24	10.3253128335000	6.5473661518000	-2.8968526249000
O25	9.5757669866000	8.9478486838000	-0.2397450694000
O26	7.7232564065000	8.8623410209000	1.7758387052000
O27	9.2122988191000	6.6265525525000	5.2925946724000
O28	16.5590726030000	1.3017983079000	2.1915342694000

TS3*

&zmat

N9	11.6541024458	3.8164525998	2.8556513090
N69	10.6722180198	7.0635434875	0.6532413790
N85	12.7244441396	6.5465533399	-0.0404361712
N93	11.0225580741	4.3958258251	2.0951201477
N101	8.5656795782	7.4960513827	1.7827962932
N109	7.5405923745	7.1053391657	2.6280163819
N117	7.7437713742	5.9846096240	3.3671783328
N125	8.9388226712	5.2404062200	3.3896894939

C21	9.7019582865	6.7030088684	1.6415813661
C29	9.8174147626	5.6407605948	2.5201082378
O37	13.8978862989	6.7839877386	0.0609008338
O53	8.4103666794	8.5726343373	1.1937011416
O61	6.8282361798	5.6138706912	4.0923179453
N77	11.9210512402	6.9710722851	1.0628581078
O45	10.3006576689	7.4039656689	-0.4892086269

d*

&zmat

N9	13.4039907415000	6.9168207264000	4.2891488949000
N69	11.7032820228000	7.3967589159000	0.4342662184000
N77	12.4294559283000	6.2638869025000	0.1781829886000
N85	11.7057971588000	5.2240650988000	0.7003431646000
N93	12.6442642802000	6.7916292296000	3.4820161327000
N101	9.5051111433000	7.8195117506000	1.6424586880000
N109	8.4984651020000	7.1611067815000	2.3066150390000
N117	8.5864994059000	5.7590987849000	2.3987463337000
N125	9.5887073398000	4.9635841947000	1.9175225203000
C21	10.5147266499000	7.0618720823000	1.0939210092000
C29	10.5023404394000	5.6891084916000	1.2870736220000
O37	12.0900277590000	4.0378228178000	0.6505937196000
O53	9.4463769694000	9.0521735342000	1.5731636607000
O61	7.6506862047000	5.2296748690000	2.9909984990000
O45	12.0961466397000	8.5312970003000	0.1012290168000

TS4*

&zmat

N69	10.8484148737	7.0712925945	0.2470054608
N77	11.9065722798	6.4717722735	-0.2538840905
N85	12.5530733359	5.5279201859	0.6536028992
N93	12.0299642199	4.9414031581	1.6842042868
N101	9.4839847282	7.5084777679	2.1012359363
N109	8.3729980055	6.6157907485	3.6777195981
N117	8.3104539014	5.4299961931	3.7583020176
N125	10.0443879994	4.6506595471	2.8782432802
C21	10.3124144174	6.6993127258	1.5566129720
C29	10.7335025783	5.3584566415	2.0829028421
O37	13.7002270454	5.2852485534	0.2717144451

O45	10.2815494654	7.9723910159	-0.3865391591
O53	9.0026141692	8.5975211481	1.9062194238
O61	7.7851440023	4.4337925969	4.1815046637

&

f*

&zmat

N69	10.5190954372000	7.1076415703000	0.2530944910000
N77	11.0130084596000	5.9356944429000	-0.1516267742000
N85	11.6124051628000	5.0679831819000	0.8679234304000
N93	11.7623061130000	5.3221968831000	2.1602157998000
N101	10.2415739878000	8.5440914838000	2.2344027530000
N109	8.4898633002000	5.1860896474000	1.7561413025000
N117	8.1642102417000	4.4592581815000	2.5854832047000
N125	11.2483212890000	7.0753911631000	3.7290410005000
C21	10.6426554832000	7.4515121461000	1.6152065021000
C29	11.2629588975000	6.5382895310000	2.5063737104000
O37	11.9929512089000	4.0068193915000	0.3855525203000
O45	9.9725724060000	7.8621867457000	-0.5635935185000
O53	10.6211978066000	8.3051710240000	3.5366302324000
O61	7.8221812283000	3.7017097581000	3.4439999217000